ON THE IMPLEMENTATION OF BOUNDARY CONDITIONS IN THE NUMERICAL SIMULATION OF MICROCHANNEL FLOWS BY DSMC METHOD

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ABSTRACT

The direct simulation Monte Carlo (DSMC) method is used to solve the 2-D steady micro-channel flows at slip flow regime and transition flow regime with Knudsen number of 0.045 and 0.108. In the DSMC method, hundreds of thousands of simulated particles are used to simulate the flow in micro-channel. The variable hard-sphere (VHS) collision model is used. A new method is proposed to modify the boundary conditions when DSMC is used to solve the low speed flow in micro-channel. The streamwise velocity distributions and nonlinear pressure distribution are obtained. The DSMC results are compared with the analytical results and they agree well each other.

INTRODUCTION

During the past decade, there have been great interests in the application of micro-dynamic devices, called MEMS (Micro-Electro-Mechanical-Systems). MEMS have become more important because of their current and potential applications in a variety of engineering problems. Most of current research work concentrates on the fabrication techniques and has made significant progress. With the success of design and fabrication techniques, there is a demand for predicting their functionality and features before they are being manufactured. Fluid effects at micron scale in MEMS play an important role in determining the features of MEMS. It is important to investigate the flow in such a small scale.

Computational methods provide powerful tools to predict and evaluate their performance by analyzing the flow feature in a system with micron size. Traditional computational fluid dynamics (CFD) is based on Navier-Stokes equations, which assume that flow is continuum. CFD methods are often inaccurate when applied to MEMS, in which the characteristic length of flow (L) approaches the molecular mean-free-path (λ), causing the continuum assumption to break down. The ratio of these two quantities is known as Knudsen number Kn ($Kn=\lambda/L$), which is used to indicate the flow rarefaction. For $Kn<0.01$, the flow is considered to be in the continuum regime and the Navier-Stokes equations are applicable. As Kn increases ($0.01<Kn<0.1$), the flow moves to "slip-flow" regime where Navier-Stokes equations can be applied by using slip velocity boundary conditions. When $0.1<Kn<3$, the flow enters "transition flow" regime, and when $Kn>3$ the flow enters the "free-molecular" regime and Boltzmann equation should be solved. The Kn number of the flow field in many MEMS often falls into the slip flow and transition flow regimes because of the extremely small device size. The small size of MEMS is a challenge to the numerical simulation tools.

The direct simulation Monte Carlo method (DSMC) is a kind of particle methods that was first used in rarefied gas dynamics by Bird[1] in the late 1960's. It has been mainly used to investigate the hypersonic flow phenomena of re-entry vehicles and the results obtained were found to be in excellent agreement with those derived from both molecular dynamics (MD) method and experiments. DSMC method is based on the Boltzmann equation, but does not solve it directly. It becomes a practical method in solving the rarefied gas phenomena. DSMC is valid when Kn number is in both 'slip flow' and 'transition flow' regimes because it avoids the continuum assumption. Compared with other particle methods such as MD method etc, DSMC method applies statistical technique to simplify the determination of collision events and hence is more efficient and feasible in practical engineering usage. It has been successfully used in rarefied gas dynamics since 1960's, and in the past five years, some attempts[2, 3] have been made to use DSMC to simulate the micro-scale flows in MEMS. In many MEMS-related flows, the characteristic length of flow is very small and comparable to the molecular mean free path so that the fluid in MEMS can be treated as "dilute fluid" and the basic binary molecular collision assumption in DSMC is reasonable.

Since micro-channel is a common element in many MEMS, it is interesting to simulate the flows in micro-channel. This paper applies DSMC method to simulate the 2-D steady flows in micro-channel at two Kn numbers (Kn=0.045, Kn=0.108), which are in the "slip flow" regime and "transition flow" regime respectively. Results are compared with some analytical solutions. The boundary conditions are modified to maintain the pressure ratio in the simulation.

IMPLEMENTATION OF BOUNDARY CONDITIONS

In traditional CFD, the boundary conditions can be clearly defined by macroscopic quantities such as velocity, temperature and pressure etc. Besides, the boundary conditions can be defined into three main categories, say, Dirichlet, Neumann and periodic boundary conditions. Unfortunately, in DSMC method, a particle-based method, it is difficult to determine such boundary conditions directly. All the macroscopic quantities should be converted to the microscopic quantities on each particle, while the macroscopic quantities will be obtained by statistical method. At inlet and outlet, particles must be introduced to represent the influence of the fluid outside the domain so that the conservation of mass and other quantities is kept.

Traditionally, most of the DSMC applications are for the simulation of hypersonic flows. Since all the characteristic lines have the same direction (in the streamwise direction) in hypersonic flows, the implementation of boundary conditions at inlet and outlet is very simple. All the variables at the inlet can be specified. At the outlet, all the variables are determined from the upstream information, and special treatment is required. However, most micro flows in MEMS are low speed flows. It is necessary to determine the variables at both inlet and outlet from inside and outside the flow field. Piekos[2] et al successfully applied characteristic line method to modify the boundary conditions. In Piekos's method, the pressure, temperature and streamwise velocity are obtained from inside the domain and only the pressure is specified at the outlet by time averaging method. This method introduces particles by mass flux instead of keeping the pressure at inlet a constant. As it does not maintain the number of particles at inlet, the pressure at the inlet may not be accurate. This paper uses a new method to modify the boundary conditions of micro-channel flow at "slip flow " regime by controlling the number of particles to maintain the pressure at both inlet and outlet.

Poiseuille flow is a pressure driven flow that involves the pressure difference along the channel. Pressure is a macroscopic quantity that can not be directly applied in DSMC method. According to the theory of ideal gas, pressure is related to the number and the temperature of molecules in a certain volume $P=nkT$, where P is pressure, n is the number of molecules in an unit volume, k is the Boltzmann constant and T is the temperature. This formulation enables us to control pressure by assigning the number of molecules in a certain volume.

The initial state in micro-channel is given such that the pressure ratio of inlet to outlet is set as 3.62. The number of particles in cells along the channel are linearly distributed with the particle number in the first cell column at inlet is as 3.62 times as that in last column at the outlet. As computation begins, the particles move along the channel. At the inlet, due to these particles moving from the cells at the first column, the particle number decreases and becomes insufficient as compared with the initial pressure. It is necessary to introduce particles from outside the flow field to sustain the pressure. The number of introduced particles can be determined by the following way. We first compute the pressure difference of each cell near the inlet between the actual pressure and the initial pressure, and then from the difference, we determine the number of particles that should be introduced. Certain number of particles is introduced from out field to keep the pressure at the inlet. At outlet, this process is also applied to maintain the outlet pressure. If the number of particles is higher, that is, the actual pressure is higher than the initial pressure, certain number of particles should be removed to keep the initial set pressure. The distributed introduced particles are put along the inlet and outlet cell column by random techniques, and the other quantities such as velocities are also assigned by random techniques. This technique will not affect the final results.

The simulation of micro-channel flow in a "slip flow" regime is selected to validate the present implementation of boundary conditions. Fig. 1 shows the pressure distribution along the channel for a micro-channel with 1.32μm height and 30μm length. The pressure ratio of inlet to outlet is set to be 3.62. It is observed from Fig. 1 that when original DSMC method is used, the streamwise pressure distribution deviates with the analytical result at inlet and outlet. Current DSMC method with present implementation of boundary conditions keeps the pressure at the inlet and outlet very well. The pressure distributions in the center part of the channel obtained by two DSMC methods have good agreement.

RESULTS AND DISCUSSION

MICRO-CHANNEL FLOW IN SLIP FLOW REGIME

The first case is a steady, 2-D flow through a micro-channel with an outlet Kn number of 0.045. This flow belongs to 'slip flow' regime that can be solved by either analytical method or DSMC method. The geometry is two parallel plates. The height of channel is 1.32μm and the length is 30μm. The pressure ratio of inlet to outlet is set to 3.62. The initial state of the gas in micro-channel is set as static and the temperature is 300K. In the present DSMC method, 240,000 particles distributed in 6,000 cells are used to simulate the flow in the computational domain so that each cell contains more than 30 particles. Each particle represents about 1.2×10^{10} molecules and the time interval Δt is $1.\times10^{-10}$. The collision model between molecules is variable hard sphere model (VHS). The collision between molecule and the walls is assumed to be diffuse reflection. The temperature on the two walls is set at 300K. In this paper, both analytical and DSMC methods are applied to obtain the solution.

Arkilic[4] et al solved Navier-Stokes equations by employing slip boundary conditions and derived the expression for analytical results of micro-channel flow in the "slip flow" regime. The streamwise slip velocity at the wall is:

$$u_w = \frac{2-\sigma}{\sigma} Kn \left.\frac{du}{dy}\right|_w \tag{1}$$

where u is the streamwise velocity, σ is the tangential accommodation coefficient. It is set as unity in this paper, in which the diffuse reflection model is applied, Kn is the Knudsen number and y is the transverse coordinate, which is zero at the center of the channel.

The analytical expression of streamwise velocity distribution is shown as below:

$$u = \frac{1}{2\mu}\frac{dp}{dx}\left[y^2 - \frac{H^2}{4} - H^2 Kn \right] \quad (2)$$

where μ is the coefficient of viscosity, p is the pressure and H is the channel height.

The analytical pressure distribution is a function of streamwise coordinate and pressure ratio:

$$P(x) = -6Kn_0 + \sqrt{(6Kn_0)^2 + (P^2 + 12Kn_0 P)(1-\frac{x}{L}) + (1+12Kn_0)\frac{x}{L}} \quad (3)$$

where P is the pressure ratio of the inlet to outlet. Kn_0 is the outlet Knudsen number, x is the coordinate in the streamwise direction.

DSMC solutions are obtained and compared with analytical results for validation. Fig.2 shows the analytical result of velocity distribution by the method of Arkilic. DSMC results presented in Fig. 3 are able to depict the flow acceleration effect. The slip velocity at wall is also obtained. Fig. 4 shows the comparisons of streamwise velocity distributions by DSMC and analytical methods at three cross-sections. There are significant differences at the positions of inlet and outlet as shown in Fig. 4a and Fig. 4c. This may be caused by the fact that the analytical method does not consider the boundary effect. In the middle part of the channel as shown in Fig. 4b, the DSMC results have good agreement with the analytical results. The pressure distributions along the channel computed by the DSMC and analytical methods are displayed in Fig. 1. From the analytical results, the streamwise velocity increases to make up the density drop caused by the pressure decrease along the channel. The velocity at walls is nonzero and increases in the streamwise direction. There still exits difference between the pressure distributions obtained by analytical method and DSMC method. This may be caused by such a reason that DSMC method considers the gas as a compressible fluid, while the analytical methods consider the fluid incompressible.

MICRO-CHANNEL FLOW IN TRANSITION FLOW REGIME

Since DSMC method does not need the continuum assumption, it is valid both in the "slip flow" regime and the "transition flow" regime. This paper uses DSMC method to investigate the flow in micro-channel in the "transition flow" regime. In the transition regime, the molecular mean free path is comparable to the characteristic dimension of the flow and Knudsen number is quite large. The analytical solution becomes inaccurate because the slip boundary condition is not valid. In contrast, DSMC method is still a feasible tool to solve this problem. A "transition flow" regime case with Knudsen number of 0.108 is simulated by DSMC method. Boundary conditions are also modified by the method introduced in this paper. The micro-channel height is 0.56μm, and the length is 30μm. Fig. 5 shows the streamwise velocity distribution obtained by DSMC method. Fig. 6 represents the streamwise velocity profile at three cross-sections at X/H=0, 27.5 and 55, respectively. From the DSMC results, it can be found that in the "transition flow" regime, the velocity distributions become flatter than that of the "slip flow" regime. Due to the rarefaction at the "transition-flow" regime which is larger than the "slip flow" regime, the flow acceleration is also greater than in the "slip flow" regime.

CONCLUSION

Micro-channel flows in the "slip flow" regime and the "transition flow" regime are simulated by direct simulation Monte Carlo method. When DSMC method is used in micro-channel flows, which are often subsonic, the boundary conditions need to be modified. By introducing particles to maintain the pressures at inlet and outlet, improved results which compare well with analytical results can be obtained, This shows that DSMC method is a feasible tool for simulating the unique flow phenomena at micro-scales. DSMC method has great promise for investigating the complicate flows in MEMS since it can simulate the flows at relatively large Knudsen number.

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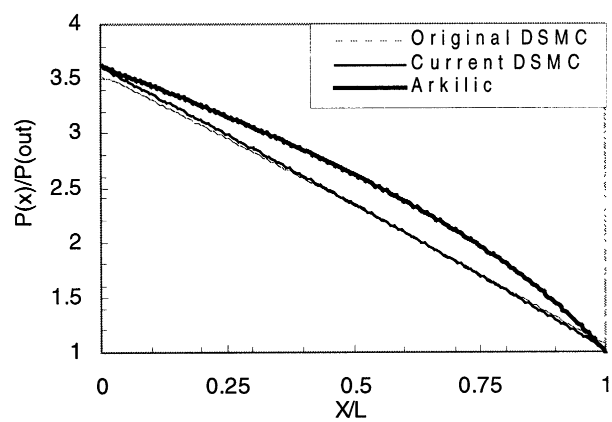

Figure 1. Streamwise pressure distributions
Kn=0.045

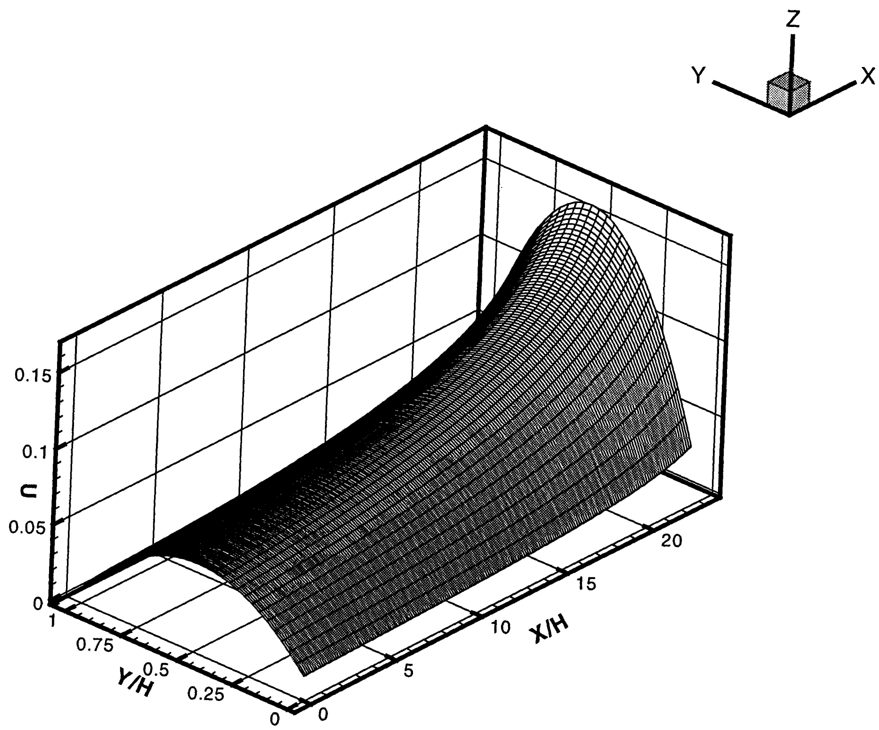

Figure 2. Analytical streamwise velocity distribution
Kn=0.045

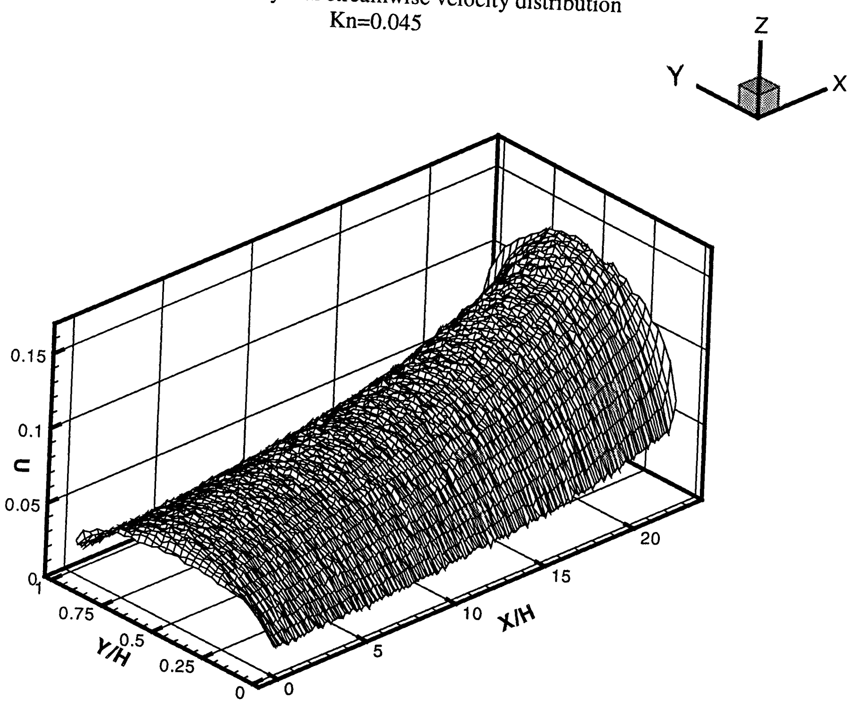

Figure 3. Streamwise velocity distribution computed by DSMC
Kn=0.045

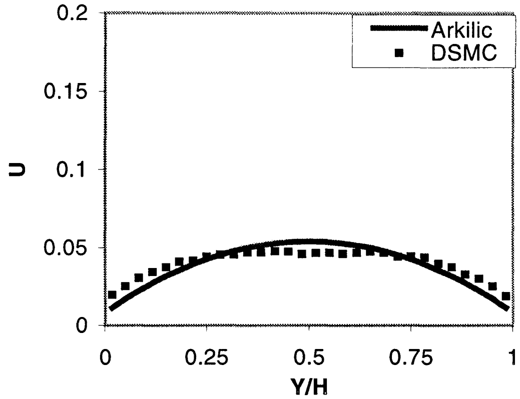

Figure 4a
Velocity profile at X/h=0, Kn=0.045

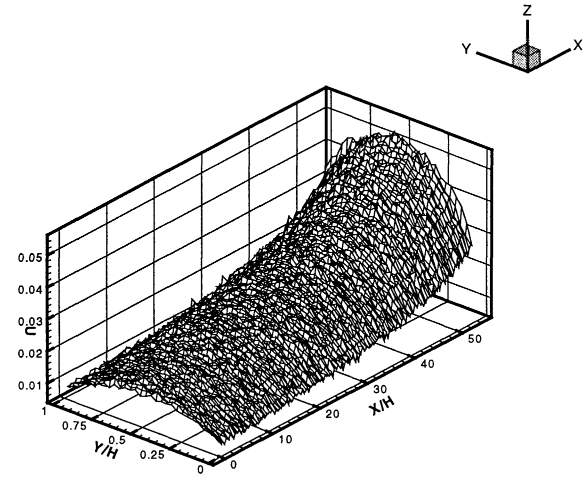

Figure 5
Streamwise velocity distribution by DSMC, Kn=0.108

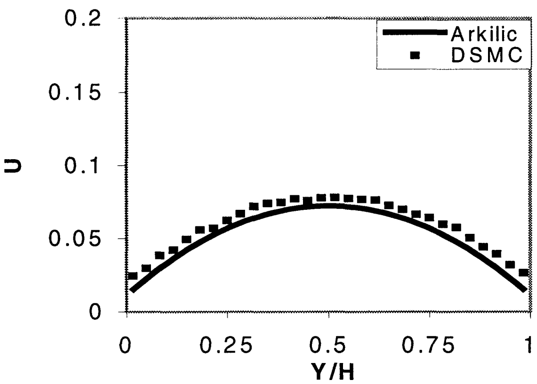

Figure 4b
Velocity profile at X/h=12, Kn=0.045

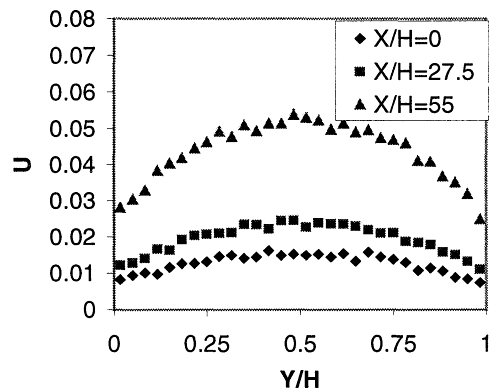

Figure 6
Velocity distributions at different cross-sections Kn=0.108

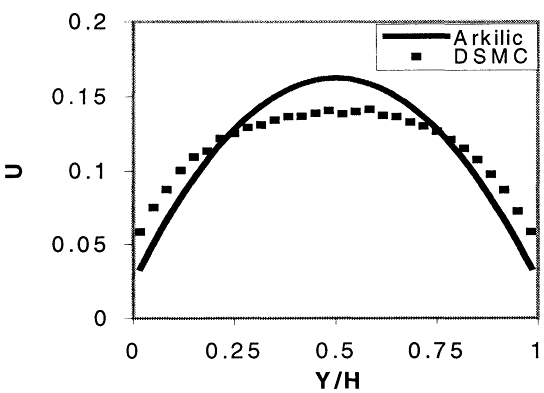

Figure 4c
Velocity profile at X/h=24, Kn=0.045

Figure 4. Comparison of computed and analytical velocity profiles at different cross-sections